



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:16 PM UTC

PDB ID : 7V53 / pdb_00007v53
Title : Crystal structure of full-length phospholipase D from Pseudomonas aeruginosa PAO1
Authors : Yang, Y.; Li, Z.
Deposited on : 2021-08-16
Resolution : 2.10 Å (reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Xtrriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

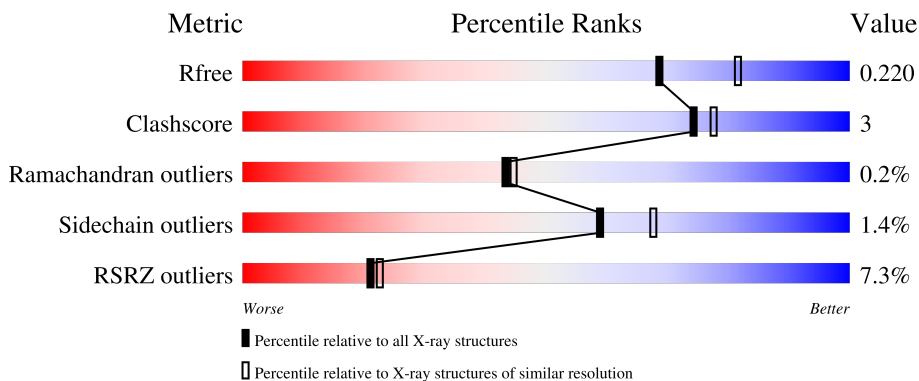
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1099	 6% 78% 7% 15%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7697 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Phospholipase D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	930	7161	4524	1281	1327	29	0	0	0

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	536	Total	O	0	0
			536	536		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	62.33Å 111.47Å 144.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	55.73 – 2.10 55.73 – 2.10	Depositor EDS
% Data completeness (in resolution range)	96.1 (55.73-2.10) 96.1 (55.73-2.10)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.31 (at 2.10Å)	Xtrriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.177 , 0.215 0.184 , 0.220	Depositor DCC
R_{free} test set	2971 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	29.0	Xtrriage
Anisotropy	0.476	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 37.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7697	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.70% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.33	0/7319	0.48	0/9948

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7161	0	6944	44	0
2	A	536	0	0	4	0
All	All	7697	0	6944	44	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (44) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1035:LEU:HD12	1:A:1036:THR:HG23	1.71	0.72
1:A:722:GLU:H	1:A:722:GLU:CD	2.02	0.68
1:A:805:PRO:O	1:A:807:GLN:N	2.34	0.60
1:A:370:GLU:OE2	1:A:373:ARG:NH1	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:354:LEU:HD22	1:A:379:LEU:HD13	1.89	0.55
1:A:561:VAL:C	1:A:562:ARG:HD2	2.33	0.54
1:A:439:ARG:NH1	1:A:443:GLU:OE1	2.42	0.53
1:A:423:LEU:O	1:A:427:MET:HG3	2.09	0.52
1:A:508:ARG:O	1:A:512:GLU:HG2	2.09	0.52
1:A:894:GLU:HG2	1:A:910:LYS:HD2	1.91	0.52
1:A:371:ALA:O	1:A:375:LYS:HG3	2.10	0.51
1:A:688:LYS:NZ	2:A:1121:HOH:O	2.42	0.50
1:A:561:VAL:O	1:A:562:ARG:HD2	2.12	0.49
1:A:190:ARG:NH2	1:A:206:ASP:OD2	2.44	0.48
1:A:374:ILE:HD13	1:A:705:LEU:HD21	1.95	0.48
1:A:1035:LEU:CD1	1:A:1036:THR:HG23	2.42	0.48
1:A:183:ILE:HD12	1:A:469:HIS:HB2	1.94	0.48
1:A:712:ALA:HA	1:A:715:TRP:CE3	2.49	0.48
1:A:517:TRP:NE1	1:A:521:LEU:HD21	2.28	0.47
1:A:116:LEU:HD23	1:A:152:ILE:CD1	2.44	0.47
1:A:744:GLN:HA	1:A:797:LYS:HE3	1.96	0.47
1:A:116:LEU:HD23	1:A:152:ILE:HD13	1.97	0.47
1:A:355:ARG:HA	1:A:355:ARG:HD3	1.60	0.47
1:A:627:ASN:HA	1:A:856:SER:O	2.16	0.46
1:A:951:GLU:H	1:A:951:GLU:CD	2.24	0.46
1:A:972:ASN:ND2	1:A:1021:GLU:OE1	2.41	0.46
1:A:566:MET:HE3	2:A:1505:HOH:O	2.16	0.45
1:A:643:ASP:HB3	1:A:1014:ARG:HE	1.82	0.45
1:A:35:PHE:CD1	1:A:45:LYS:HD2	2.51	0.45
1:A:79:GLY:HA2	1:A:168:GLN:O	2.17	0.45
1:A:609:LYS:HB2	1:A:878:LEU:HB3	2.00	0.43
1:A:961:LYS:HE2	2:A:1568:HOH:O	2.16	0.43
1:A:764:ASN:HB3	1:A:1025:TYR:CZ	2.54	0.43
1:A:35:PHE:HA	1:A:889:MET:HE3	1.99	0.43
1:A:899:ARG:O	1:A:946:ILE:HG22	2.19	0.43
1:A:195:PHE:CZ	1:A:922:LYS:HE2	2.54	0.42
1:A:562:ARG:HG3	2:A:1515:HOH:O	2.20	0.42
1:A:348:PRO:O	1:A:352:ARG:NH1	2.53	0.42
1:A:133:VAL:HG11	1:A:148:CYS:HB2	2.02	0.41
1:A:152:ILE:H	1:A:152:ILE:HG12	1.69	0.41
1:A:857:LYS:HD3	1:A:870:SER:HA	2.02	0.41
1:A:203:ARG:HB3	1:A:447:PRO:HG3	2.03	0.41
1:A:614:LEU:HD23	1:A:614:LEU:C	2.46	0.40
1:A:368:LEU:HB3	1:A:372:LEU:HD12	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	920/1099 (84%)	895 (97%)	23 (2%)	2 (0%)	43 44

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	25	PRO
1	A	805	PRO

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	731/910 (80%)	721 (99%)	10 (1%)	59 67

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	SER
1	A	29	ILE
1	A	152	ILE
1	A	349	GLU
1	A	355	ARG
1	A	363	THR
1	A	501	LEU
1	A	695	THR
1	A	705	LEU

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Mol	Chain	Res	Type
1	A	856	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	382	GLN
1	A	491	GLN
1	A	691	GLN
1	A	744	GLN
1	A	793	GLN
1	A	1018	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	930/1099 (84%)	0.09	68 (7%) 21 22	19, 30, 70, 96	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	537	LEU	3.8
1	A	541	LEU	3.7
1	A	498	THR	3.5
1	A	346	ILE	3.3
1	A	396	ILE	3.3
1	A	1011	GLY	3.2
1	A	803	SER	3.1
1	A	518	LEU	3.1
1	A	1010	PRO	3.0
1	A	698	ARG	3.0
1	A	29	ILE	3.0
1	A	330	ILE	3.0
1	A	544	PRO	3.0
1	A	804	ASP	3.0
1	A	530	TYR	3.0
1	A	545	THR	2.9
1	A	395	LEU	2.8
1	A	806	ALA	2.8
1	A	538	ARG	2.8
1	A	30	SER	2.7
1	A	347	GLU	2.7
1	A	543	PRO	2.6
1	A	510	ALA	2.6
1	A	394	THR	2.6
1	A	378	LEU	2.6
1	A	529	ASN	2.6
1	A	500	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	523	ALA	2.6
1	A	354	LEU	2.6
1	A	379	LEU	2.6
1	A	993	PHE	2.5
1	A	384	MET	2.5
1	A	366	LEU	2.5
1	A	805	PRO	2.5
1	A	531	LEU	2.5
1	A	361	LEU	2.5
1	A	389	LEU	2.5
1	A	521	LEU	2.5
1	A	539	LEU	2.4
1	A	350	LEU	2.4
1	A	506	LEU	2.4
1	A	417	GLY	2.4
1	A	801	GLY	2.4
1	A	383	TRP	2.4
1	A	517	TRP	2.4
1	A	26	CYS	2.4
1	A	336	LEU	2.4
1	A	380	ILE	2.4
1	A	532	ASP	2.3
1	A	348	PRO	2.3
1	A	372	LEU	2.3
1	A	525	ALA	2.3
1	A	1015	ALA	2.3
1	A	1013	LEU	2.2
1	A	509	SER	2.2
1	A	699	GLN	2.2
1	A	341	LEU	2.2
1	A	1035	LEU	2.1
1	A	342	ASP	2.1
1	A	524	ALA	2.1
1	A	368	LEU	2.1
1	A	421	TRP	2.1
1	A	387	THR	2.1
1	A	499	PRO	2.1
1	A	329	SER	2.1
1	A	369	PRO	2.0
1	A	693	PRO	2.0
1	A	142	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.